WHAT IS CLAIMED IS:

1. A composition comprising a polypeptide comprising a SUMO protease catalytic domain in a trapped proteolytic deacylation intermediate complex with its substrate.

2. The composition of claim 1, wherein the complexed molecules have a crystalline structure.

3. The composition of claim 1, wherein the SUMO protease is Ulp1.

4. The composition of claim 3, wherein the substrate is Smt3.

5. The composition of claim 3, wherein the polypeptide consists of the catalytic domain of Ulp1.

6. The composition of claim 2, wherein the complex has crystal structure coordinates as shown in Table 1.

7. A method of forming a complex of a polypeptide comprising a catalytic domain of a protease with its substrate, which method comprises:

(a) combining the protease with its substrate in a molar ratio to produce a mixture;

(b) adding a reducing agent capable of trapping a proteolytic deacylation intermediate complex of the protease and the substrate in amount effective to trap an isolatable amount of the complex; and

(c) adjusting the pH of the mixture to about 7.0.

8. The method of claim 7, wherein steps (a) and (b) are performed simultaneously.

9. The method of claim 7, wherein the pH is adjusted to about 7.0 by dialyzing the mixture.

10. The method of claim 9, further comprising isolating the complex after dialysis.

11. The method of claim 9, wherein the protease is a SUMO protease.

12. The method of claim 7 where the protease is a polypeptide comprising a catalytic domain of Ulp1

13. The method of claim 12 where the substrate is Smt3.

14. The method of claim 13 where Ulp1 and Smt3 are present in a molar ratio from 1:1 to 1:5.

15. The method of claim 14 where Ulp1 and Smt3 are present in a molar ratio of 1:3.

16. The method of claim 7, wherein the reducing agent is sodium borohydride.

17. A polynucleotide comprising a sequence, wherein the sequence encodes a mutant Ulp1.

18. The polynucleotide of claim 17, wherein the mutant Ulp1 comprises the amino acid sequence shown in SEQ ID NO:2, but contains an amino acid substitution at a position selected from the group consisting of 432, 448, 451, 455, 472, 474, 489, 490, 493, and 515.

19. A recombinant vector comprising the polynucleotide sequence of claim 17.

20. The recombinant vector of claim 19, where the polynucleotide encodes a mutant Ulp1 comprising an amino acid substitution at position 432, 448, 451, 455, 472, 474, 489, 490, 493, and/or 515.

21. A host cell comprising the recombinant vector of claim 19.

22. A host cell comprising the recombinant vector of claim 20.

23. A process of producing mutant Ulp1, comprising culturing the host cell of claim 21 under conditions whereby the polynucleotide encoding the mutant Ulp1 is expressed.

24. A mutant Ulp1 polypeptide.

25. The polypeptide of claim 24, wherein the mutant Ulp1 comprising an amino acid substitution at position 432, 448, 451, 455, 472, 474, 489, 490, 493, and/or 515 of SEQ ID NO: 2.

26. A method of identifying potential substrates of a cysteine protease by rational drug design, which method comprises designing candidate substrates that would form interactions with catalytic site amino acids identified from computer modeling based on the crystal structure of the composition of claim 2.

27. The method according to claim 26, wherein the crystal structure has a catalytic site having crystal structure coordinates as shown in Table 1.

28. The method according to claim 26, which further comprises synthesizing the candidate substrate and determining whether the candidate substrate interacts with the cysteine protease.

29. The method according to claim 26, wherein the candidate substrate is a cysteine protease inhibitor.

30. The method of claim 26, wherein the protease is Ulp1.